## REMARKS

Claims 1-19 are pending in the application. The Examiner has rejected claims 1-6. With this response, Applicants have amended claims 1, 2, 3, 6, 7, 9, 10, and 11-16, have canceled claim 8, and have new claims 17-21. Applicants respectfully submit that no new matter is presented with these amendments or new claim, and respectfully submit that claims 1-7 and 9-21 are in condition for allowance.

### *I. Restriction Requirement:*

Applicants hereby affirm the election of Group I, without traverse, which includes claims 1-6 (in part), drawn to a compound of formula I, wherein Q is pyrimidinyl (or A is N), classified in class 544, subclasses 330, 331, 333. Claim 1 has been amended so that only the elected subject matter is encompassed by the scope of the claims. Applicants reserve the right, however, to pursue the non-elected subject matter in future continuation or divisional applications.

Pending the allowance of claims 1-6 (in part), Applicants request the rejoinder of originally filed claims 7 through 16, pursuant to MPEP §821.04. Specifically, Applicants request that the process claims that depend from or otherwise include all the limitations of the patentable product be entered. In anticipation of said rejoinder, and to expedite the prosecution process, Applicants have also presented (and, for certain of these claims, amended or cancelled) claims 7 through 16 below. Applicants have also added new claims 17-19 which also include all of the limitations of claim 1 and respectfully request that these new claims be considered with the rejoined claims.

### *II. Rejection under 35 U.S.C. § 112, second paragraph:*

a) The Examiner has rejected claim 1 and states that the term "aliphatic group" is indefinite because the specification does not clearly define the term and appears to even read on aromatic rings since it includes unsaturated cyclic hydrocarbons. In response to the Examiner's rejection and to further clarify claim 1, Applicants have amended the definition of the term "aliphatic" in the specification to clarify that aromatic rings are not included in the definition of aliphatic. As defined in the specification, aliphatic groups may have one or more units of unsaturation (e.g., alkenyl groups); however Applicants have clarified the definition to ensure

that aromatic rings are not included within the definition of aliphatic. In response to the Examiner's assertion that the accepted meaning for "aliphatic group" is "straight or branched chain arrangement" Applicants respectfully disagree. Applicants respectfully submit that the term "aliphatic" is also often defined as including cyclic moieties. Applicants submit herewith the following four documents reciting the definition of "aliphatic" as specifically including cyclic moieties within the scope of the term.

| | |
|---|---|
| Exhibit 1. | IUPAC Compendium of Chemical Terminology |
| Exhibit 2. | Glossary of Class Names of Organic Compounds and Reactive Intermediates Based on Structure (IUPAC Recommendations) |
| Exhibit 3. | The IUPAC Systematic Approach to Nomenclature |
| Exhibit 4. | Handbook of Organic Chemistry |

Applicants respectfully point out to the Examiner that the International Union of Pure and Applied Chemistry (IUPAC) defines the term "aliphatic" as "acyclic or cyclic, saturated or unsaturated carbon compounds, excluding aromatic compounds." (*See* Exhibits 1 and 2). Furthermore, the IUPAC rules to nomenclature specifically recites that "The alkanes and cycloalkanes are also members of a larger class of compounds referred to as aliphatic. Simply put, aliphatic compounds are compounds that do not incorporate any aromatic rings in their molecular structure." (*See* Exhibit 3). Moreover, the Handbook of Organic Chemistry, at Table 8-11, recites various unsaturated aliphatic hydrocarbons as including such cyclic groups as 1,4-cyclohedadiene, cyclohexene, and 1,3,5,7-cyclooctatetraene. (*See* Exhibit 4).

As recited in the M.P.E.P. at § 706.03(d) ¶ 7.34.02, "While applicant may be his or her own lexicographer, a term in a claim may not be given a meaning repugnant to the usual meaning of that term." Applicants respectfully submit that although the term "aliphatic" is defined at times as only including straight chain hydrocarbon moieties, it is also defined as including cyclic moieties. Applicants further submit that because the IUPAC definition of the term "aliphatic" includes cyclic hydrocarbon moieties, then Applicants' definition of the term "aliphatic" as cannot be considered "repugnant" to its usual meaning. Accordingly, Applicants respectfully submit that the term aliphatic, as defined in the specification (and now amended to clearly state aromatic rings are not included), is indeed definite and request that the Examiner withdraw her rejection of claim 1 35 U.S.C. § 112, second paragraph.

b) The Examiner has rejected claims 2 and 3 and states that the claims lack antecedent

basis for reciting "-$CH_2$(substituted heterocylcyl), and "substituted heterocyclyl" and states that they are not recited for the definition of $R^2$ in claim 1. Applicants respectfully disagree and submit that claim 1 includes the definition of both –$CH_2$(heterocyclyl) and heterocyclyl, and that heterocyclyl, as defined in the specification may be optionally substituted with one or more more substituents. For example, as stated in the specification starting on page 11 aryl and non-aromatic heterocyclic rings may be substituted:

"An aryl group (carbocyclic and heterocyclic) or an aralkyl group, such as benzyl or phenethyl, may contain one or more substituents. Examples of suitable substituents on the unsaturated carbon atom of an aryl group include a halogen, -R, -OR, -OH, -SH, -SR, protected OH (such as acyloxy), phenyl (Ph), substituted Ph, -OPh, substituted -OPh, -$NO_2$, -CN, -$NH_2$, -NHR, -$N(R)_2$, -NHCOR, -NHCONHR, -NHCON$(R)_2$, -NRCOR, -$NHCO_2R$, -$CO_2R$, -$CO_2H$, -COR, -CONHR, -CON$(R)_2$, -S$(O)_2$R, -$SONH_2$, -S(O)R, -$SO_2$NHR, or -NHS$(O)_2$R, where R is an aliphatic group or a substituted aliphatic group.

An aliphatic group or a non-aromatic heterocyclic ring may contain one or more substituents. Examples of suitable substituents on the saturated carbon of an aliphatic group or of a non-aromatic heterocyclic ring include those listed above for the unsaturated carbon, such as in an aromatic ring, as well as the following: =O, =S, =NNHR, =$NNR_2$, =N-OR, =NNHCOR, =$NNHCO_2R$, =$NNHSO_2R$, or =NR.

A substitutable nitrogen on an aromatic or non-aromatic heterocyclic ring may be optionally substituted. Suitable substituents on the nitrogen include R, COR, S$(O)_2$R, and $CO_2R$, where R is an aliphatic group or a substituted aliphatic group."

Thus, Applicants respectfully submit that the terms used in claims 2 and 3 do indeed fall within the scope of claim 1, and as dependent claims, further define a specific embodiment of the invention (e.g., substituted heterocyclyl groups).

c) The Examiner has rejected claim 4 and states that the claim lacks antecedent basis for reciting "benzyloxymethyl" and states that the group "-$CH_2$OR" does not cover "benzyloxymethyl" because R is an "aliphatic group". In response to the Examiner's rejection, Applicants have amended claim 3 to include –$CH_2$aryl- (as defined in claim 1), and thus Applicants respectfully submit that claim 4 (after amendment of claim 3) does indeed fall within

the scope of claim 3.

d) The Examiner has rejected claims 4 and 5 and states that they lack antecedent basis for reciting the limitation of "wherein each of $R^1$-$R^3$ is optionally substituted" and states that this phrase is not recited in claim 3 (or ultimately claim 1). Applicants respectfully disagree with the Examiner and submit that claim 1 and claim 3 both include substituents that are optionally substituted as defined generally in the specification. As defined in the specification starting on page 11:

"An aryl group (carbocyclic and heterocyclic) or an aralkyl group, such as benzyl or phenethyl, may contain one or more substituents. Examples of suitable substituents on the unsaturated carbon atom of an aryl group include a halogen, -R, -OR, -OH, -SH, -SR, protected OH (such as acyloxy), phenyl (Ph), substituted Ph, -OPh, substituted -OPh, $-NO_2$, -CN, $-NH_2$, -NHR, $-N(R)_2$, -NHCOR, -NHCONHR, $-NHCON(R)_2$, -NRCOR, $-NHCO_2R$, $-CO_2R$, $-CO_2H$, -COR, -CONHR, $-CON(R)_2$, $-S(O)_2R$, $-SONH_2$, -S(O)R, $-SO_2NHR$, or $-NHS(O)_2R$, where R is an aliphatic group or a substituted aliphatic group.

An aliphatic group or a non-aromatic heterocyclic ring may contain one or more substituents. Examples of suitable substituents on the saturated carbon of an aliphatic group or of a non-aromatic heterocyclic ring include those listed above for the unsaturated carbon, such as in an aromatic ring, as well as the following: =O, =S, =NNHR, $=NNR_2$, =N-OR, =NNHCOR, $=NNHCO_2R$, $=NNHSO_2R$, or =NR.

A substitutable nitrogen on an aromatic or non-aromatic heterocyclic ring may be optionally substituted. Suitable substituents on the nitrogen include R, COR, $S(O)_2R$, and $CO_2R$, where R is an aliphatic group or a substituted aliphatic group."

Thus, Applicants respectfully submit that the term "wherein each of $R^1$-$R^3$ is optionally substituted" used in claims 4 and 5 does indeed fall within the scope of claim 1, and that claims 4 and 5, as dependent claims, further define a specific embodiment of the invention (e.g., "wherein each of $R^1$-$R^3$ is optionally substituted").

e) The Examiner has rejected claim 6 and states that it is not certain which compounds of Table 1 are intended. In response to the Examiner's rejection, Applicants have amended claim 6 to include specific compounds.

***III. Additional Remarks:***

As detailed above, Applicants have amended claim 1 to exclude certain compounds disclosed in WO00/31063 (as cited in the International Search Report and in the IDS submitted December 2, 2002) where:

"when G is hydrogen, and $R^2$ is optionally substituted phenyl, then $R^3$ is not hydrogen"

Applicants have also added certain of the new claims (20 and 21) directed to certain additional embodiments, support for which can be found throughout the specification and in the compounds disclosed in Table 1.

**CONCLUSION**

Applicants respectfully submit that in view of the foregoing amendments and remarks, claims 1-21 are in condition for allowance. Applicants would like to thank the Examiner for careful consideration of the above-referenced case. If it is believed that a telephone call would expedite prosecution, the Examiner is invited to contact the undersigned at (617) 444-6536. The Commissioner is also authorized to charge any fees (or credit any overpayments) to Deposit Account Number: 50-0725, reference number VPI/00-126 US.

Respectfully submitted,

Karoline KMS

Dated 12/23/03

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# IUPAC Compendium of Chemical Terminology

1-1 of 1 items

aliphat: 1

**aliphatic compounds**
IUPAC Compendium of Chemical Terminology aliphatic compounds Acyclic or cyclic, saturated or unsaturated carbon compounds, excluding aromatic compounds. 1995, 67, 1313 IUPAC Compendium of Chemical Terminology 2nd Edition (1997) ...
**author:** A D McNaught & A Wilkinson **subject:** IUPAC Compendium of Chemical Terminology **Score:** 100% **updated:** 11/09/1998
**matching:** aliphat

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# IUPAC Compendium of Chemical Terminology

## search

This online version of the IUPAC Compendium of Chemical Terminology corresponds to the second edition, compiled by Alan D. McNaught and Andrew Wilkinson (Royal Society of Chemistry, Cambridge, UK) and published in print form by Blackwell Science in 1997. Some minor errors have been corrected (the changes are noted where they occur), and cross-referencing has been improved. The conversion to electronic form was carried out by David Stout (Information Technology Consultant, Information Services, Royal Society of Chemistry).

The Compendium is popularly referred to as the "Gold Book", in recognition of the contribution of the late Victor Gold, who initiated work on the first edition. It is one of the series of IUPAC "Colour Books" on chemical nomenclature, terminology, symbols and units (see the list of source documents), and collects together terminology definitions from IUPAC recommendations already published in *Pure and Applied Chemistry* and in the other Colour Books.

Terminology definitions published by IUPAC are drafted by international committees of experts in the appropriate chemistry sub-disciplines, and ratified by IUPAC's Interdivisional Committee on Nomenclature and Symbols. In this edition of the Compendium these IUPAC-approved definitions are supplemented with some definitions from ISO and from the International Vocabulary of Basic and General Terms in Metrology; both these sources are recognised by IUPAC as authoritative. The result is a collection of nearly 7000 terms, with authoritative definitions, spanning the whole range of chemistry.

All IUPAC recommendations published up to the end of 1995 were considered for inclusion, together with some particularly significant material published in 1996 (class names, kinetics, clinical chemistry quantities and units, stereochemistry, photochemistry and basic polymer terms). A selection was made on the basis of general utility: some terms were omitted as being of interest only to a highly specialist audience.

Some minor editorial changes were made to the originally published definitions, to harmonis th pres ntation and to clarify their applicability, if this is limited to a particular sub-discipline. Verbal definitions of terms from Quantities, Units and Symbols in Physical Chemistry (the IUPAC Green Book, in which definitions are generally given as mathematical expressions)

were developed specially for this Compendium by the Physical Chemistry Division of IUPAC. Definitions of a few physicochemical terms not mentioned in the Green Book were added at the same time (referred to here as Physical Chemistry Division, unpublished).

The first reference given at the end of each definition is to the page of *Pure Appl. Chem.* or other source where the original definition appears; other references given designate other places where compatible definitions of the same term or additional information may be found, in other IUPAC documents. The complete reference citations are given in the appended list of source documents. Highlighted terms within individual definitions link to other entries where additional information is available.

A cross (+) against an entry implies that use of the term is discouraged.

Please send any comments by e-mail to Alan McNaught at the Royal Society of Chemistry: adm@rsc.org.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
ORGANIC CHEMISTRY DIVISION
COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY
COMMISSION ON PHYSICAL ORGANIC CHEMISTRY

# GLOSSARY OF CLASS NAMES OF ORGANIC COMPOUNDS AND REACTIVE INTERMEDIATES BASED ON STRUCTURE

## (IUPAC Recommendations 1994)

**http://www.chem.qmul.ac.uk/iupac/class/**

Prepared for publication by: G. P. Moss, P. A. S. Smith, D. Tavernier.

Composition of the Joint Working Party (1980-1994): H. J. T. Bos, A. J. Boulton, E. W. Godly, P. Grünanger, A. D. McNaught, G. P. Moss, R. Panico, J. Rigaudy, P. A. S. Smith (*Convenor*), J. H. Stocker, D. Tavernier, (from Commission III.1); R. A. Y. Jones, J. March, J. M. McBride, P. Müller (*Convenor*) (from Commission III.2).

**World Wide Web version Prepared by G. P. Moss**

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The definitions used in this glossary are identical to those in the published document, see G.P. Moss, P.A.S. Smith and D. Tavernier, *Pure and Applied Chemistry*, **67**, 1307-1375 (1995) [Copyright IUPAC; reproduced with the permission of IUPAC]. If you use any of these definitions please cite this reference as their source.

For problems in converting the text into a World Wide Web version see the IUPAC home page.

Any comments, corrections or suggestions for additional entries in a future edition should be e-mailed to g.p.moss@qmul.ac.uk

As well as an Introduction all class names included are listed alphabetically in the following files: A; B; C; D,E; F,G; H; I; K,L; M; N; O; P; Q,R; S; T; U-Z. Each class name then leads to a file of definitions of class names of related substances. These in turn may lead to other files from cross-references. Related classes are grouped together under the following headings.

1. **Carbon, Hydrogen and Oxygen**:
   - Acyclic Hydrocarbons
   - Ring systems
   - Alcohols, Ethers, Phenols and Derivatives
   - Aldehydes, Ketones, Quinones and Derivatives (See also oximes, azines, etc. under Nitrogen)

- Carboxylic acids and derivatives (See also amides, amidines, etc. under Nitrogen)

2. **Based on Other Elements**:
    - Boron
    - Halogens
    - Metals
    - Nitrogen (one N atom only)
    - Nitrogen (two or more N atoms)
    - Phosphorus, Arsenic, Antimony and Bismuth
    - Silicon, Germanium, Tin and Lead
    - Sulfur, Selenium and Tellurium
3. **Natural Products**:
    - Antibiotics (β-lactams and tetracyclins)
    - Carbohydrates (and cyclitols)
    - Lipids
    - Nucleic acids and component units
    - Terpenoids including retinoids and steroids
    - Tetrapyrroles and related compounds
    - Others natural products
4. **Others**:
    - Ions and Radicals
    - Miscellaneous.

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Return to main IUPAC Chemical Nomenclature home page

# Acyclic Hydrocarbons

Quick move to entries starting with the letters C, D, H, O, P, or V.

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**acetylenes:**

Acyclic (branched or unbranched) and cyclic (with or without side chain) *hydrocarbons* having one or more carbon-carbon triple bonds. See also *alkynes*.

**acetylides:***

Compounds arising by replacement of one or both hydrogen atoms of acetylene (ethyne) by a metal or other cationic group. E.g. NaC≡CH monosodium acetylide. NOC Rule C-84.3. By extension, analogous compounds derived from terminal *acetylenes*, RC≡CH.

**aliphatic compounds:**

Acyclic or cyclic, saturated or unsaturated carbon compounds, excluding *aromatic compounds.*

**alkanes:***

Acyclic branched or unbranched *hydrocarbons* having the general formula $C_nH_{2n+2}$, and therefore consisting entirely of hydrogen atoms and saturated carbon atoms. NOC Rule A-1.1. Cf. *cycloalkanes*.

**alkanium ions:**

*Carbocations* derived from *alkanes* by C-hydronation containing at least one pentacoordinate carbon atom. RNRI Rule RC-82.1.1.2. Cf. *carbonium ions.* E.g. $^{+}CH_5$ methanium, $[C_2H_7]^{+}$ ethanium.

**alkenes:***

Acyclic branched or unbranched *hydrocarbons* having one carbon-carbon double bond and the general formula $C_nH_{2n}$ . Acyclic branched or unbranched hydrocarbons having more than one double bond are alkadienes, alkatrienes, etc. NOC Rule A-3.1. See also *olefins.*

**alkyl groups:***

Univalent groups derived from *alkanes* by removal of a hydrogen atom from any carbon atom: $C_nH_{2n+1}$-. The groups derived by removal of a hydrogen atom from a terminal carbon atom of unbranched alkanes form a subclass of normal alkyl (*n*-alkyl) groups: $H[CH_2]_n$-. NOC Rule A-1.2. The groups $RCH_2$-, $R_2CH$- (R not equal to H), and $R_3C$- (R not equal to H) are primary, secondary and tertiary alkyl groups respectively. See also *cycloalkyl groups*. Cf. *hydrocarbyl groups*.

**alkyl radicals:***

Carbon-centered radicals derived formally by removal of one hydrogen atom from an *alkane*. RNRI Rule RC-81.1.1. E.g. $CH_3CH_2CH_2^{\cdot}$ propyl.

**alkylenes**:

1. An old term, which is not recommended, for *alkenes*, especially those of low molecular weight.

2. An old term for alkanediyl groups commonly but not necessarily having the free valencies on adjacent carbon atoms. E.g. $-CH(CH_3)CH_2-$ propylene (systematically called propane-1,2-diyl).

**alkylidenes:***

*Carbenes* $R_2C$: formed by mono or dialkyl substitution of methylene, $H_2C$: RNRI Rule RC-81.1.3. E.g. $CH_3CH_2CH$: propylidene.

**alkylidene groups:***

The divalent groups formed from *alkanes* by removal of two hydrogen atoms from the same carbon atom, the free valencies of which are part of a double bond. GNOC Recom. R-2.5. E.g. $(CH_3)_2C=$ propan-2-ylidene.

**alkylidynes:***

*Carbenes* $RC\vdots$ formed by alkyl substitution of methyne, $HC\vdots$ RNRI Rule RC-81.1.3. E.g. $CH_3CH_2C\vdots$ propylidyne.

**alkynes:***

Acyclic branched or unbranched *hydrocarbons* having a carbon-carbon triple bond and the general formula $C_nH_{2n-2}$ , $RC{\equiv}CR$. Acyclic branched or unbranched hydrocarbons having more than one triple bond are known as alkadiynes, alkatriynes, etc. NOC Rule A-3.2. See also *acetylenes*.

**allenes:**

*Hydrocarbons* (and by extension, derivatives formed by substitution) having two double bonds from one carbon atom to two others: $R_2C{=}C{=}CR_2$. (The simplest member, propadiene, is known as allene.) See also *cumulenes*, *dienes*.

**allylic groups**:

The group $CH_2{=}CHCH_2-$ (allyl) and derivatives formed by substitution. The term 'allylic position' or 'allylic site' refers to the saturated carbon atom. A group, such as -OH, attached at an allylic site is sometimes described as 'allylic'.

**allylic intermediates**:

*Carbanions*, *carbenium ions*, or *radicals*, formally derived by detachment of one hydron, hydride or hydrogen from the $CH_3$ group of propene or derivatives thereof. E.g. $H_2C{=}CHCH_2^+$ allyl cation.

**cumulenes:***

*Hydrocarbons* (and by extension, derivatives formed by substitution) having three or more cumulative double bonds. E.g. $R_2C{=}C{=}C{=}CR_2$. (Cumulative double bonds are those present in a chain in which at least three

contiguous atoms are joined by double bonds.) NOC Rule A-21.1, footnote. See also *allenes*, *heterocumulenes*.

**dienes:**

Compounds that contain two fixed double bonds (usually assumed to be between carbon atoms). See *alkenes*, *olefins*. Dienes in which the two double-bond units are linked by one single bond are termed conjugated, e.g. $CH_2$=CH-CH=$CH_2$ buta-1,3-diene. Dienes in which the double bonds are adjacent are called cumulative, e.g. $CH_3$CH=C=$CH_2$ buta-1,2-diene. See also *allenes*, *cumulenes*. Those in which one or more of the unsaturated carbon atoms is replaced by a heteroatom may be called heterodienes.

**hydrocarbons:**

Compounds consisting of carbon and hydrogen only.

**olefins:**

Acyclic and cyclic *hydrocarbons* having one or more carbon-carbon double bonds, apart from the formal ones in *aromatic compounds*. The class olefins subsumes *alkenes* and cycloalkenes and the corresponding polyenes. See also *cycloalkanes*.

**paraffins:**

Obsolescent term for saturated *hydrocarbons*, commonly but not necessarily acyclic. Still widely used in the petrochemical industry, where the term designates acyclic saturated hydrocarbons, and stands in contradistinction to *naphthenes*.

**vinylic groups:**

The vinyl group ($CH_2$=CH-) and derivatives formed by substitution. Informally, a group, such as -OH, attached to the free valence of a (substituted) vinyl group is sometimes referred to as 'vinylic'.

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# Nomenclature

# Naming Organic Compounds

The increasingly large number of organic compounds identified with each passing day, together with the fact that many of these compounds are isomers of other compounds, requires that a systematic nomenclature system be developed. Just as each distinct compound has a unique molecular structure which can be designated by a structural formula, each compound must be given a characteristic and unique name.
As organic chemistry grew and developed, many compounds were given trivial names, which are now commonly used and recognized. Some examples are:

| **Name** | Methane | Butane | Acetone | Toluene | Acetylene | Ethyl Alcohol |
|---|---|---|---|---|---|---|
| **Formula** | $CH_4$ | $C_4H_{10}$ | $CH_3COCH_2$ | $CH_3C_6H_5$ | $C_2H_2$ | $C_2H_5OH$ |

Such **common names** often have their origin in the history of the science and the natural sources of specific compounds, but the relationship of these names to each other is arbitrary, and no rational or systematic principles underly their assignments.

## The IUPAC Systematic Approach to Nomenclature

A rational nomenclature system should do at least two things. First, it should indicate how the carbon atoms of a given compound are bonded together in a characteristic lattice of chains and rings. Second, it should identify and locate any functional groups present in the compound. Since hydrogen is such a common component of organic compounds, its amount and locations can be assumed from the tetravalency of carbon, and need not be specified in most cases.
The IUPAC nomenclature system is a set of logical rules devised and used by organic chemists to circumvent problems caused by arbitrary nomenclature. Knowing these rules and given a structural formula, one should be able to write a unique name for every distinct compound. Likewise, given a IUPAC name, one should be able to write a structural formula. In general, an IUPAC name will have three essential features:

- A root or base indicating a major chain or ring of carbon atoms found in the molecular structure.
- A suffix or other element(s) designating functional groups that may be present in the compound.
- Names of substituent groups, other than hydrogen, that complete the molecular structure.

As an introduction to the IUPAC nomenclature system, we shall first consider compounds that have no specific functional groups. Such compounds are composed only of carbon and hydrogen atoms bonded together by sigma bonds (all carbons are $sp^3$ hybridized).

An xcell nt presentation of organic nomenclature is provided on a Nomenclature Page. created by

Dave Woodcock.
A full presentation of the IUPAC Rules is also available.

## Alkanes

# Alkanes

Hydrocarbons having no double or triple bond functional groups are classified as **alkanes** or **cycloalkanes**, depending on whether the carbon atoms of the molecule are arranged only in chains or also in rings. Although these hydrocarbons have no functional groups, they constitute the framework on which functional groups are located in other classes of compounds, and provide an ideal starting point for studying and naming organic compounds. The alkanes and cycloalkanes are also members of a larger class of compounds referred to as **aliphatic**. Simply put, aliphatic compounds are compounds that do not incorporate any aromatic rings in their molecular structure.
The following table lists the IUPAC names assigned to simple continuous-chain alkanes from C-1 to C-10. A common "ane" suffix identifies these compounds as alkanes. Longer chain alkanes are well known, and their names may be found in many reference and text books. The names **methane** through **decane** should be memorized, since they constitute the root of many IUPAC names. Fortunately, common numerical prefixes are used in naming chains of five or more carbon atoms.

| Name | Molecular Formula | Structural Formula | Isomers | Name | Molecular Formula | Structural Formula | Isomers |
|---|---|---|---|---|---|---|---|
| methane | $CH_4$ | $CH_4$ | 1 | hexane | $C_6H_{14}$ | $CH_3(CH_2)_4CH_3$ | 5 |
| ethane | $C_2H_6$ | $CH_3CH_3$ | 1 | heptane | $C_7H_{16}$ | $CH_3(CH_2)_5CH_3$ | 9 |
| propane | $C_3H_8$ | $CH_3CH_2CH_3$ | 1 | octane | $C_8H_{18}$ | $CH_3(CH_2)_6CH_3$ | 18 |
| butane | $C_4H_{10}$ | $CH_3CH_2CH_2CH_3$ | 2 | nonane | $C_9H_{20}$ | $CH_3(CH_2)_7CH_3$ | 35 |
| pentane | $C_5H_{12}$ | $CH_3(CH_2)_3CH_3$ | 3 | decane | $C_{10}H_{22}$ | $CH_3(CH_2)_8CH_3$ | 75 |

**Some important behavior trends and terminologies:**

(i) The formulas and structures of these alkanes increase uniformally by a $CH_2$ increment.
(ii) A uniform variation of this kind in a series of compounds is called **homologous**.
(iii) These formulas all fit the $C_nH_{2n+2}$ rule. This is also the highest possible H/C ratio for a stable hydrocarbon.
(iv) Since the H/C ratio in these compounds is at a maximum, we call them **saturated** (with hydrog n).

Beginning with butane ($C_4H_{10}$), and becoming more numerous with larger alkanes, we not the

existence of alkane isomers. For example, there are five $C_6H_{14}$ isom rs, shown below as abbr viated line formulas (**A** through **E**):

**A** **B** **C** **D** **E**

Although these distinct compounds all have the same molecular formula, only one (**A**) can be called hexane. How then are we to name the others?

The **IUPAC** system requires first that we have names for simple unbranched chains, as noted above, and second that we have names for simple alkyl groups that may be attached to the chains. Examples of some common **alkyl groups** are given in the following table. Note that the "ane" suffix is replaced by "**yl**" in naming groups. The symbol **R** is used to designate a generic (unspecified) alkyl group.

| **Group** | $CH_3$- | $C_2H_5$- | $CH_3CH_2CH_2$- | $(CH_3)_2CH$- | $CH_3CH_2CH_2CH_2$- | $(CH_3)_2CHCH_2$- | $CH_3CH_2CH(CH_3)$- | $(CH_3)_3C$- | F |
|---|---|---|---|---|---|---|---|---|---|
| **Name** | Methyl | Ethyl | Propyl | Isopropyl | Butyl | Isobutyl | sec-Butyl | tert-Butyl | Al |

## IUPAC Rules for Alkane Nomenclature

1. Find and name the longest continuous carbon chain.
2. Identify and name groups attached to this chain.
3. Number the chain consecutively, starting at the end nearest a substituent group.
4. Designate the location of each substituent group by an appropriate number and name.
5. Assemble the name, listing groups in alphabetical order.
   The prefixes di, tri, tetra etc., used to designate several groups of the same kind, are not cons alphabetizing.

For the above isomers of hexane the IUPAC names are: **B** 2-methylpentane **C** 3-methylpentane **D** 2,2-dimethylbutane **E** 2,3-dimethylbutane

**Halogen substituents** are easily accomodated, using the names: fluoro (F-), chloro (Cl-), bromo (Br-) and iodo (I-). For example, $(CH_3)_2CHCH_2CH_2Br$ would be named 1-bromo-3-methylbutane. If the halogen is bonded to a simple alkyl group an alternative "alkyl halide" name may be used. Thus, $C_2H_5Cl$ may be named chloroethane (no locator number is needed for a two carbon chain) or ethyl chloride.

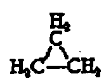
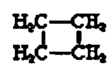
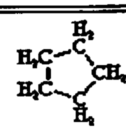
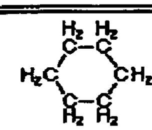
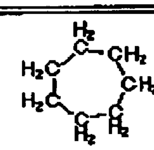
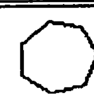
For additional examples of how these rules are used in naming branched alkanes, and for some sub-rules of nomenclature [redacted].

Cycl alkanes

# Cycloalkanes

**Cycloalkanes** have one or more rings of carbon atoms. The simplest examples of this class consist of a single, unsubstituted carbon ring, and these form a homologous series similar to the unbranched alkanes. The IUPAC names of the first five members of this series are given in the following table. The last (yellow shaded) column gives the general formula for a cycloalkane of any size. If a simple unbranched alkane is converted to a cycloalkane two hydrogen atoms, one from each end of the chain, must be lost. Hence the general formula for a cycloalkane composed of **n** carbons is $C_nH_{2n}$.

### Examples of Simple Cycloalkanes

| Name | Cyclopropane | Cyclobutane | Cyclopentane | Cyclohexane | Cycloheptane | Cyc |
|---|---|---|---|---|---|---|
| Molecular Formula | $C_3H_6$ | $C_4H_8$ | $C_5H_{10}$ | $C_6H_{12}$ | $C_7H_{14}$ | ( |
| Structural Formula |  |  |  |  |  | ( |
| Line Formula |  |  |  |  |  | < |

Substituted cycloalkanes are named in a fashion very similar to that used for naming branched alkanes. The chief difference in the rules and procedures occurs in the numbering system. Since all the carbons of a ring are equivalent (a ring has no ends like a chain does), the numbering starts at a substituted ring atom.

### IUPAC Rules for Cycloalkane Nomenclature

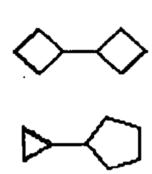
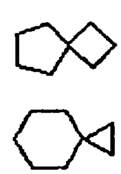
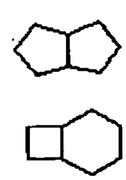
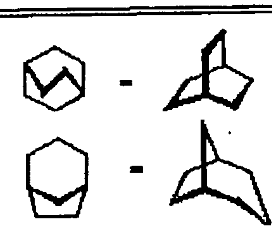
1. For a monosubstituted cycloalkane the ring supplies the root name (table above) and the su named as usual. A location number is unnecessary.
2. If the alkyl sustituent is large and/or complex, the ring may be named as a substituent grouṛ
3. If two different substituents are present on the ring, they are listed in alphabetical order, and substituent is assigned to carbon #1. The numbering of ring carbons then continues in a directio counter-clockwise) that affords the second substituent the lower possible location number.
4. If several substituents are present on the ring, they are listed in alphabetical order. Location assigned to the substituents so that one of them is at carbon #1 and the other locations have the numbers, counting in either a clockwise or counter-clockwise direction.
5. The name is assembled, listing groups in alphabetical order and giving each group (if there a location number. The pr fixes di, tri, t tra etc., used to designate several groups of the same k consid red when alphabetizing.

For examples of how thes rules are used in naming substituted cycloalkanes [redacted].

Small rings, such as three and four membered rings, have significant angle strain resulting from the distortion of the sp[3] carbon bond angles from the ideal 109.5° to 60° and 90° respectively. This angle strain often enhances the chemical reactivity of such compounds, leading to ring cleavage products. It is also important to recognize that, with the exception of cyclopropane, cycloalkyl rings are not planar (flat). The three dimensional shapes assumed by the common rings (especially cyclohexane and larg r rings) are described and discussed in the Conformational Analysis Section.

Hydrocarbons having more than one ring are common, and are referred to as **bicyclic** (two rings), **tricyclic**(three rings) and in general, **polycyclic** compounds. The molecular formulas of such compounds have H/C ratios that decrease with the number of rings. In general, for a hydrocarbon composed of **n carbon atoms** associated with **m rings** the formula is: $C_nH_{(2n+2-2m)}$. The structural relationship of rings in a polycyclic compound can vary. They may be separate and independent, or they may share one or two common atoms. Some examples of these possible arrangements are shown in the following table.

### Examples of Isomeric $C_8H_{14}$ Bicycloalkanes

| Isolated Rings | Spiro Rings | Fused Rings | Bridged Rings |
|---|---|---|---|
| No common atoms | One common atom | One common bond | Two common atoms |
|  |  |  |  |

### Practice Problems

Choose a Problem

### Alkenes & Alkynes

# Alken s and Alkyn s

Alkenes and alkynes ar hydrocarbons which respectively have **carbon-carbon double bond** and **carbon-carbon tripl bond** functional groups. Th molecular formulas of th se **unsaturated**

hydrocarbons refl ct th multipl bonding of the functional groups:

| | | | |
|---|---|---|---|
| **Alkane** | R-$CH_2$-$CH_2$-R | $C_nH_{2n+2}$ | This is the maximum H/C ratio for a given number of carbon atoms. |
| **Alkene** | R-CH=CH-R | $C_nH_{2n}$ | Each double bond reduces the number of hydrogen atoms by 2. |
| **Alkyne** | R-C≡C-R | $C_nH_{2n-2}$ | Each triple bond reduces the number of hydrogen atoms by 4. |

As noted earlier in the Analysis of Molecular Formulas section, the molecular formula of a hydrocarbon provides information about the possible structural types it may represent. For example, consider compounds having the formula $C_5H_8$. The formula of the five-carbon alkane pentane is $C_5H_{12}$ so the difference in hydrogen content is 4. This difference suggests such compounds may have a triple bond, two double bonds, a ring plus a double bond, or two rings. Some examples are shown here, and there are at least fourteen others!

$H_3C—C≡C–CH_2–CH_3$ $H_2C=CH–CH_2–CH=CH_2$ 

## IUPAC Rules for Alkene and Cycloalkene Nomenclature

1. The **ene** suffix (ending) indicates an alkene or cycloalkene.
2. The longest chain chosen for the root name must include both carbon atoms of the double b
3. The root chain must be numbered from the end nearest a double bond carbon atom. If the c center of the chain, the nearest substituent rule is used to determine the end where numbering s
4. The smaller of the two numbers designating the carbon atoms of the double bond is used a: locator. If more than one double bond is present the compound is named as a diene, triene or e( indicating the number of double bonds, and each double bond is assigned a locator number.
5. In cycloalkenes the double bond carbons are assigned ring locations #1 and #2. Which of tl determined by the nearest substituent rule.
6. Substituent groups containing double bonds are:
   **$H_2C$=CH-** Vinyl group
   **$H_2C$=CH-$CH_2$-** Allyl group

## IUPAC Rules for Alkyne Nomenclature

1. Th **yn** suffix (ending) indicates an alkyne or cycloalkyne.
2. The longest chain chos n for the root name must includ both carbon atoms of th triple bo
3. Th root chain must be numbered from the end nearest a triple bond carbon atom. If the trip

center of the chain, the near st substituent rule is used to determine the nd wh re numbering s

4. The smaller of the two numbers designating the carbon atoms of the triple bond is used as t locator.

5. If several multiple bonds are present, each must be assigned a locator number. Double bon bonds in the IUPAC name, but the chain is numbered from the end nearest a multiple bond, regi

6. Because the triple bond is linear, it can only be accomodated in rings larger than ten carbon cycloalkynes the triple bond carbons are assigned ring locations #1 and #2. Which of the two is : determined by the nearest substituent rule.

7. Substituent groups containing triple bonds are:

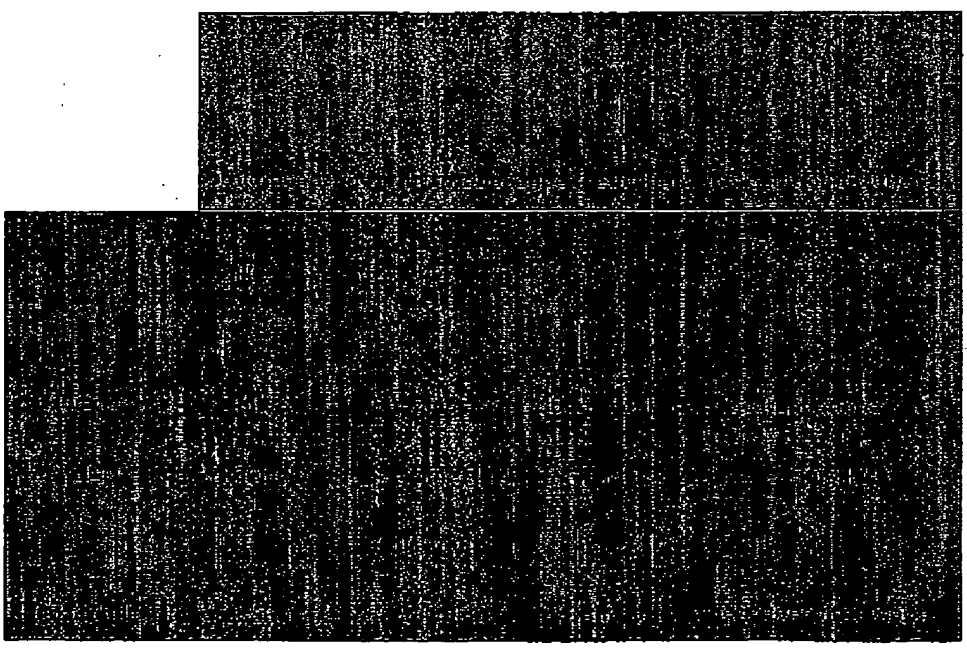
   **HC≡C-** Ethynyl group
   **HC≡CH-$CH_2$-** Propargyl group

For examples of how these rules are used in naming alkenes, alkynes and cyclic analogs [redacted]

**Benzene Derivatives**

# Benzene Derivatives

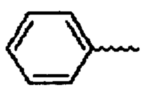
The nomenclature of substituted benzene ring compounds is less systematic than that of the alkanes, alkenes and alkynes. A few mono-substituted compounds are named by using a group name as a prefix to "benzene", as shown by the combined names listed below. A majority of these compounds, however, are referred to by singular names that are unique. There is no simple alternative to memorization in mastering these names.



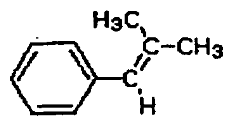
**Combined Names**

**Singular Names**

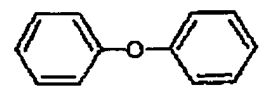
Two commonly encountered substituent groups that incorporate a benz ne ring are **phenyl**, abbreviated Ph-, and **benzyl**, abbreviated Bn-. These are shown here with examples of their use. Be careful not to confuse a phenyl (pronounced *fenyl*) group with the compound phenol (pronounced *feenol*). A general and useful generic notation that complements the use of **R-** for an alkyl group is **Ar-** for an aryl group (any aromatic ring).



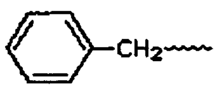
Phenyl Group



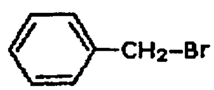

2-methyl-1-phenylpropene



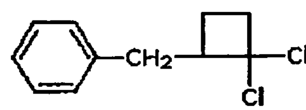

diphenyl ether




Benzyl Group

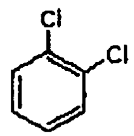



benzyl bromide

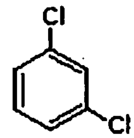



2-benzyl-1,1-dichlorocyclobutane

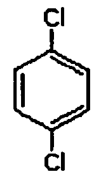
When more than one substituent is present on a benzene ring, the relative locations of the substituents must be designated by numbering the ring carbons or by some other notation. In the case of disubstituted benzenes, the prefixes *ortho, meta & para* are commonly used to indicate a 1,2- or 1,3- or 1,4- relationship respectively. In the following examples, the first row of compounds show this usage in red. Some disubstituted toluenes have singular names (e.g. xylene, cresol & toluidine) and their isomers are normally designated by the ortho, meta or para prefix. A few disubstituted benzenes have singular names given to specific isomers (e.g. salicylic acid & resorcinol). Finally, if there are three or more substituent groups, the ring is numbered in such a way as to assign the substituents the lowest possible numbers, as illustrated by the last row of examples. The substituents are listed alphabetically in the final name. If the substitution is symmetrical (third example from the left) the numbering corresponds to the alphabetical order.



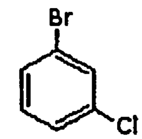
1,2-dichlorobenzene
*ortho*-dichlorobenzene
*o*-dichlorobenzene



1,3-dichlorobenzene
*meta*-dichlorobenzene
*m*-dichlorobenzene

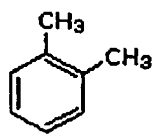


1,4-dichlorobenzene
*para*-dichlorobenzene
*p*-dichlorobenzene

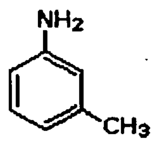


1-bromo-3-chlorobenzene
*meta*-chlorobromobenzene
*m*-chlorobromobenzene

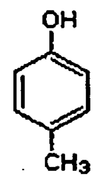
2-brom
*ortho*-b
*o*-brom



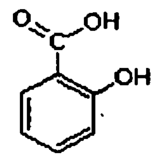
1,2-dimethylbenzene
*ortho*-xylene
*o*-xylene



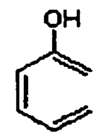
3-aminotoluene
*meta*-toluidine
*m*-toluidine



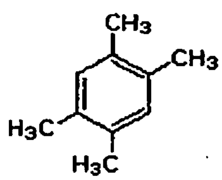
4-hydroxytoluene
*para*-cresol
*p*-cresol



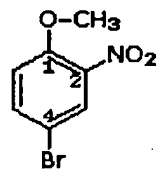
*o*-hydroxybenzoic acid
salicylic acid



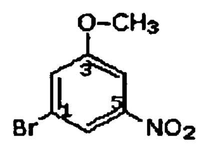
1,3-dihydrox
resorci



1,2,4,5-tetramethylbenzene
durene



4-bromo-1-methoxy-2-nitrobenzene



1-bromo-3-methoxy-5-nitrobenzene

2,4-dichlor

## Practice Problems

Five questions concerning nomenclature are presented here.

Choose a Problem

**Return to Table of Contents**

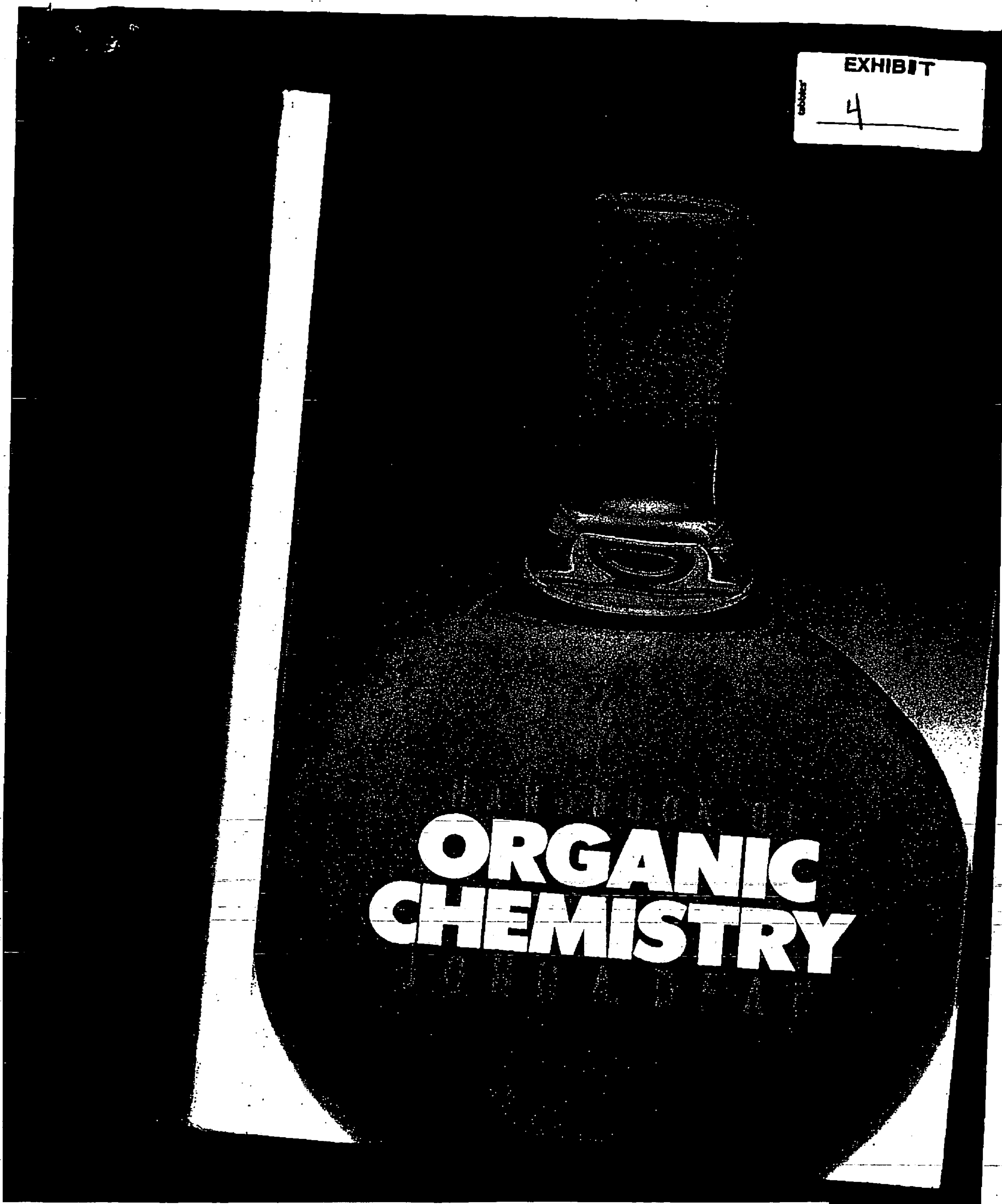


EXHIBIT
4
ORGANIC
CHEMISTRY

**TABLE 8-11 Half-wave potentials (vs. saturated calomel electrode) of organic compounds at 25°C**

The solvent systems in this table are listed below:

- A acetonitrile and a perchlorate salt such as $LiClO_4$ or a tetraalkyl ammonium salt
- B acetic acid and an alkali acetate, often plus a tetraalkyl ammonium iodide
- C 0.05 to 0.175 *M* tetraalkyl ammonium halide and 75% 1,4-dioxane
- D buffer plus 50% ethanol (EtOH)

*Abbreviations Used in the Table*

Bu, butyl; Et, ethyl; EtOH, ethanol; *M*, molar; Me, methyl; MeOH, methanol; PrOH, propanol

| Compound | Solvent system | $E_{1/2}$ |
|---|---|---|
| **Unsaturated aliphatic hydrocarbons** | | |
| Acrylonitrile | C but 30% EtOH | −1.94 |
| Allene | C | −2.29 |
| 1,3-Butadiene | A | −2.03 |
| | C | −2.59 |
| 1,3-Butadiyne | C | −1.89 |
| 1-Buten-2-yne | C | −2.40 |
| 1,4-Cyclohexadiene | A | −1.6 |
| Cyclohexene | A | −1.89 |
| 1,3,5,7-Cyclooctatetraene | B | −1.42 |
| | C | −1.51 |
| Diethyl fumarate | B, pH 4.0 | −0.84 |
| Diethyl maleate | B, pH 4.0 | −0.95 |
| 2,3-Dimethyl-1,3-butadiene | A | −1.83 |
| Dimethylfulvene | C | −1.89 |
| Diphenylacetylene | C | −2.20 |
| 1,1-Diphenylethylene | B | −1.52 |
| | C | −2.19 |
| Ethyl methacrylate | 0.1 *N* LiCl+25% EtOH | −1.9 |
| 2-Methyl-1,3-butadiene | A | −1.84 |
| 2-Methyl-1-butene | A | −1.97 |
| 1-Piperidino-4-cyano-4-phenyl-1,3-butadiene | $LiClO_4$ in dimethylformamide | −0.16 |
| *trans*-Stilbene | B | −1.51 |
| Tetrakis(dimethylamino)ethylene | A | −0.75 |
| **Aromatic hydrocarbons** | | |
| Acenaphthene | A | −0.95 |
| | B | −1.36 |
| | C | −2.58 |
| Anthracene | A | −0.84 |
| | B | −1.20 |
| | C | −1.94 |

ELECTR

TABLE 8-11 compounds at

Co

Azulene
1,2-Benzanthrace
2,3-Benzanthrace
Benzene
1,2-Benzo[*a*]pyre
Biphenyl
Chrysene
1,2,5,6-Dibenzanth
1,2-Dihydronaphth
9,10-Dimethylanth
2,3-Dimethylnapht
9,10-Diphenylanthr
Fluorene
Hexamethylbenzene
Indan
Indene
1-Methylnaphthalene
2-Methylnaphthalene
Naphthalene
Pentamethylbenzene
Phenanthrene
Phenylacetylene
Pyrene
*trans*-Stilbene
Styrene